

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046158.D
 Acq On : 07 Dec 2021 22:33
 Operator : SY/MD
 Sample : M4960-06 10X
 Misc : 6.25g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 42 Sample Multiplier: 1

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M

Title : VOC Analysis

Signal : TIC: VU046168.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	74	81	93	rVB	113110	125838	14.75%	1.804%
2	1.919	171	180	196	rVB	80343	102608	12.03%	1.471%
3	2.215	267	272	276	rVB2	406	383	0.04%	0.005%
4	2.340	308	311	317	rVB2	250	265	0.03%	0.004%
5	2.572	369	383	413	rBV	184698	310349	36.38%	4.449%
6	2.790	449	451	456	rVB	194	174	0.02%	0.002%
7	2.935	494	496	499	rBV	154	131	0.02%	0.002%
8	2.970	502	507	511	rVB3	356	329	0.04%	0.005%
9	3.051	523	532	542	rVB3	1638	2993	0.35%	0.043%
10	3.189	558	575	595	rBV2	13315	32443	3.80%	0.465%
11	3.314	606	614	617	rBB	211	282	0.03%	0.004%
12	3.340	617	622	627	rBB	194	274	0.03%	0.004%
13	3.417	641	646	647	rBV	153	132	0.02%	0.002%
14	3.491	667	669	676	rBV	152	211	0.02%	0.003%
15	3.556	686	689	691	rBV	142	121	0.01%	0.002%
16	3.639	711	715	719	rBV	156	199	0.02%	0.003%
17	3.729	740	743	745	rBV	178	146	0.02%	0.002%
18	3.900	793	796	798	rBV	162	140	0.02%	0.002%
19	4.163	874	878	881	rBB	159	156	0.02%	0.002%
20	4.301	917	921	927	rBB	151	228	0.03%	0.003%
21	4.639	1010	1026	1068	rBV	73744	229931	26.95%	3.296%
22	4.848	1088	1091	1095	rVB2	360	310	0.04%	0.004%
23	4.871	1095	1098	1101	rBV	328	291	0.03%	0.004%
24	4.906	1106	1109	1111	rVV	225	131	0.02%	0.002%
25	5.067	1142	1159	1180	rBV	141445	323869	37.96%	4.643%
26	5.199	1197	1200	1201	rBV	243	140	0.02%	0.002%
27	5.289	1225	1228	1230	rVB	230	151	0.02%	0.002%
28	5.388	1255	1259	1261	rBB	191	157	0.02%	0.002%
29	5.449	1275	1278	1283	rBV	169	215	0.03%	0.003%
30	5.543	1305	1307	1311	rBV	141	146	0.02%	0.002%
31	5.594	1319	1323	1327	rBV	171	221	0.03%	0.003%
32	5.729	1342	1365	1386	rVV2	318570	853170	100.00%	12.231%
33	5.970	1436	1440	1443	rBV2	686	731	0.09%	0.010%
34	6.121	1484	1487	1493	rBV2	299	321	0.04%	0.005%
35	6.250	1512	1527	1555	rBV	284950	543382	63.69%	7.790%
36	6.420	1577	1580	1583	rVV2	232	172	0.02%	0.002%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

37	6.436	1583	1585	1588	rVB	242	159	0.02%	0.002%
38	6.459	1589	1592	1595	rBB2	255	185	0.02%	0.003%
39	6.530	1605	1614	1631	rVV4	4156	8371	0.98%	0.120%
40	6.633	1642	1646	1649	rBV	181	202	0.02%	0.003%
41	6.694	1649	1665	1687	rVV	191280	367751	43.10%	5.272%
42	6.864	1715	1718	1721	rBV	165	161	0.02%	0.002%
43	7.044	1769	1774	1777	rBV2	243	261	0.03%	0.004%
44	7.182	1814	1817	1820	rBV2	216	160	0.02%	0.002%
45	7.279	1845	1847	1851	rBV	121	133	0.02%	0.002%
46	7.417	1887	1890	1893	rBB	142	119	0.01%	0.002%
47	7.494	1910	1914	1917	rBV	154	182	0.02%	0.003%
48	7.568	1923	1937	1954	rBV	109052	188482	22.09%	2.702%
49	7.684	1969	1973	1980	rVB2	415	487	0.06%	0.007%
50	7.790	1997	2006	2014	rBV2	1426	2320	0.27%	0.033%
51	7.899	2025	2040	2056	rBV	415440	715697	83.89%	10.260%
52	8.179	2116	2127	2145	rBV	74524	122998	14.42%	1.763%
53	8.247	2145	2148	2151	rVV2	369	300	0.04%	0.004%
54	8.395	2191	2194	2196	rBV	157	132	0.02%	0.002%
55	8.452	2209	2212	2216	rBV	114	126	0.01%	0.002%
56	8.475	2216	2219	2222	rVV2	199	147	0.02%	0.002%
57	8.636	2256	2269	2301	rBV	242669	453429	53.15%	6.500%
58	8.915	2348	2356	2367	rBV4	2528	4103	0.48%	0.059%
59	9.263	2459	2464	2465	rBV	197	199	0.02%	0.003%
60	9.330	2479	2485	2488	rBV	165	247	0.03%	0.004%
61	9.417	2499	2512	2538	rBV	407021	673359	78.92%	9.653%
62	9.568	2555	2559	2561	rBV2	259	226	0.03%	0.003%
63	9.690	2593	2597	2605	rBV2	767	988	0.12%	0.014%
64	9.803	2628	2632	2634	rBV2	231	189	0.02%	0.003%
65	9.909	2661	2665	2670	rVB	161	138	0.02%	0.002%
66	9.983	2679	2688	2692	rBV	109	187	0.02%	0.003%
67	10.063	2709	2713	2718	rVB2	147	140	0.02%	0.002%
68	10.671	2895	2902	2909	rVB3	2579	3290	0.39%	0.047%
69	10.758	2917	2929	2947	rVB	281557	451636	52.94%	6.475%
70	10.838	2950	2954	2957	rBV	208	151	0.02%	0.002%
71	10.867	2958	2963	2967	rBV3	293	282	0.03%	0.004%
72	10.922	2977	2980	2981	rBV	234	152	0.02%	0.002%
73	11.095	3029	3034	3037	rBV2	192	229	0.03%	0.003%
74	11.115	3037	3040	3042	rBV2	412	281	0.03%	0.004%
75	11.208	3066	3069	3072	rBV	266	146	0.02%	0.002%
76	11.375	3119	3121	3127	rVB2	204	208	0.02%	0.003%

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Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF Filtering: 5
 Sampling : 1 Min Area: 0 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

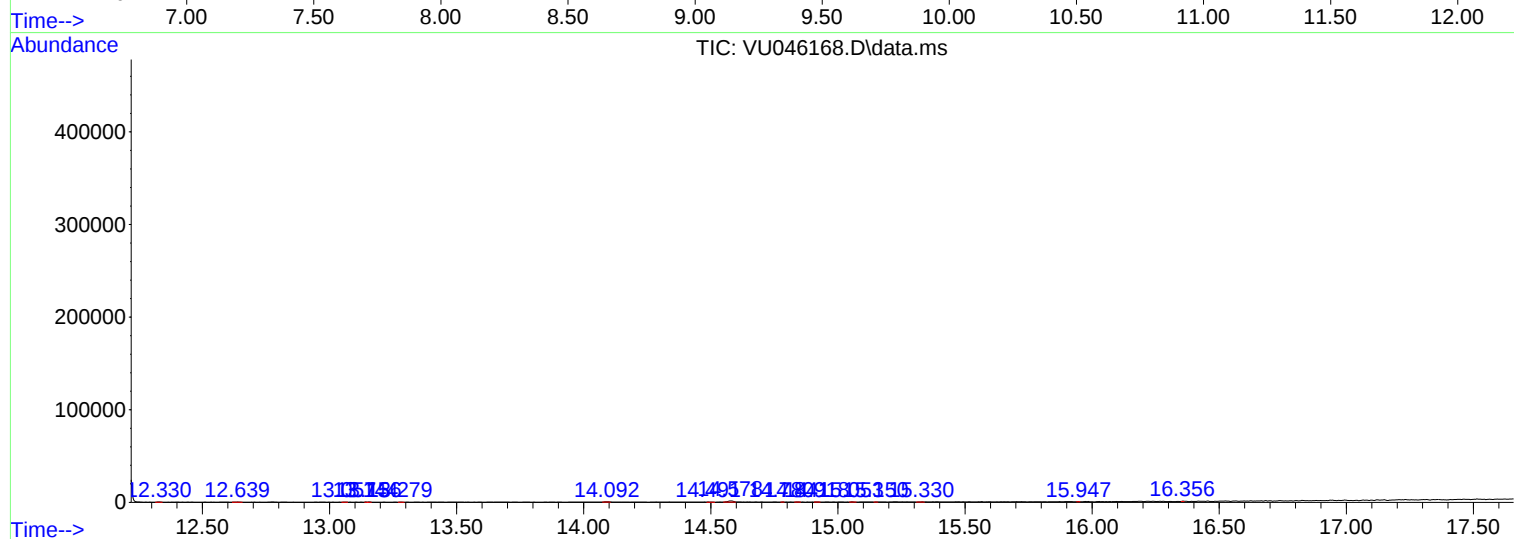
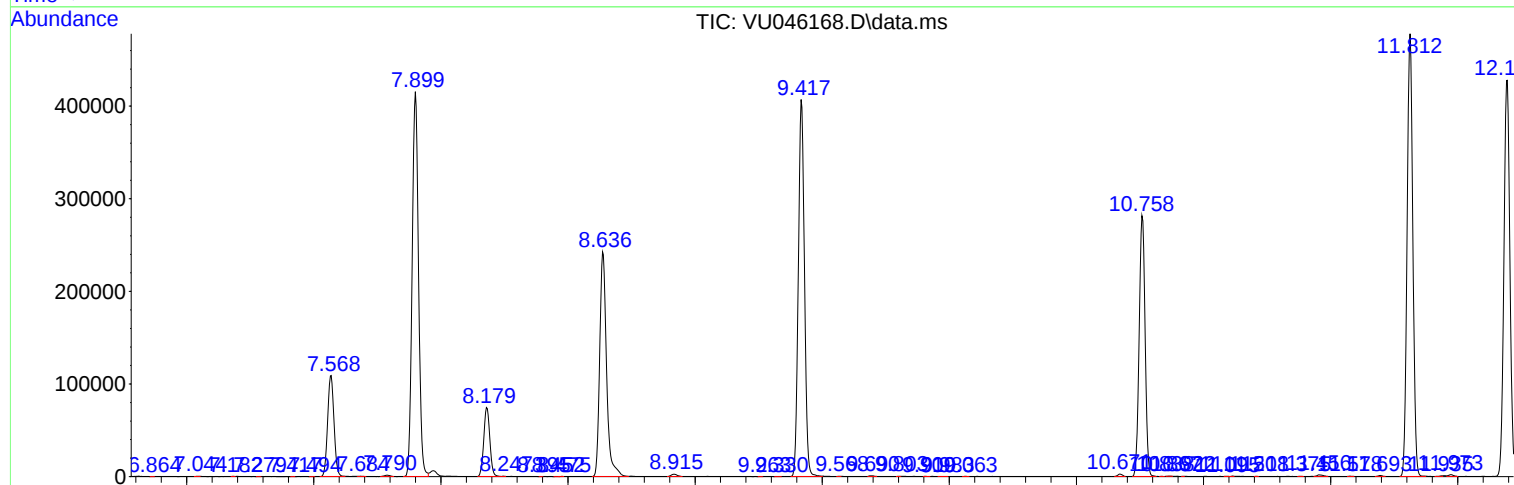
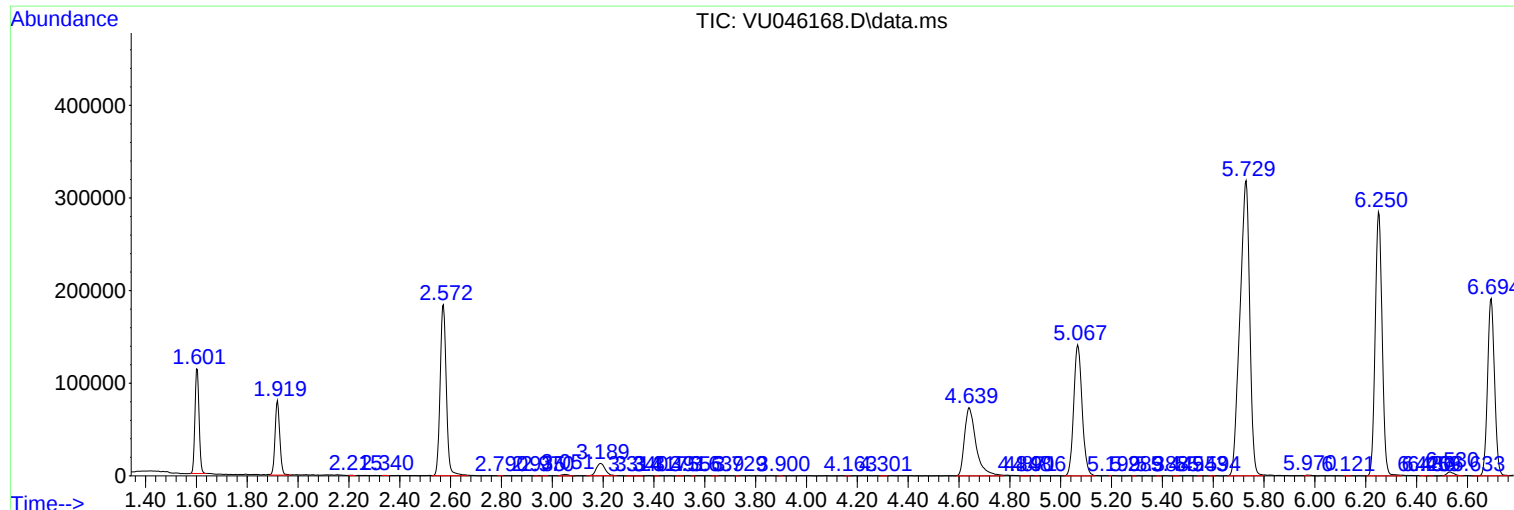
77	11.456	3139	3146	3157	rVB3	1757	2977	0.35%	0.043%
78	11.578	3180	3184	3189	rVV	369	325	0.04%	0.005%
79	11.693	3214	3220	3227	rVV4	1025	1230	0.14%	0.018%
80	11.812	3244	3257	3276	rBV	477939	740205	86.76%	10.611%
81	11.935	3287	3295	3297	rBV2	594	628	0.07%	0.009%
82	11.973	3302	3307	3316	rVB3	1957	2643	0.31%	0.038%
83	12.195	3360	3376	3395	rBV	427634	692763	81.20%	9.931%
84	12.330	3413	3418	3422	rBV3	404	371	0.04%	0.005%
85	12.639	3507	3514	3520	rBV2	330	401	0.05%	0.006%
86	13.057	3641	3644	3649	rBV	206	153	0.02%	0.002%
87	13.144	3669	3671	3673	rVV	322	201	0.02%	0.003%
88	13.156	3673	3675	3678	rVB	388	218	0.03%	0.003%
89	13.279	3710	3713	3718	rBV	130	132	0.02%	0.002%
90	14.092	3960	3966	3970	rBV2	411	506	0.06%	0.007%
91	14.491	4088	4090	4098	rVB	282	256	0.03%	0.004%
92	14.578	4108	4117	4123	rBV2	1292	1975	0.23%	0.028%
93	14.780	4178	4180	4183	rBV2	250	140	0.02%	0.002%
94	14.841	4195	4199	4203	rBV2	216	218	0.03%	0.003%
95	14.918	4219	4223	4227	rBV2	277	258	0.03%	0.004%
96	15.053	4262	4265	4271	rVB2	325	316	0.04%	0.005%
97	15.150	4292	4295	4297	rBV2	180	121	0.01%	0.002%
98	15.330	4344	4351	4354	rBV	353	505	0.06%	0.007%
99	15.947	4540	4543	4545	rBV2	309	178	0.02%	0.003%
100	16.356	4668	4670	4672	rBV2	362	189	0.02%	0.003%

Sum of corrected areas: 6975602

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ALS Vial : 42 Sample Multiplier: 1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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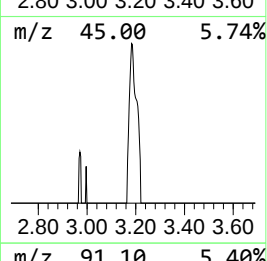
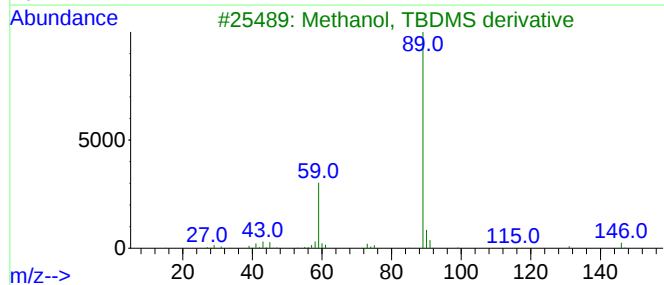
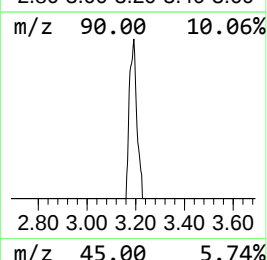
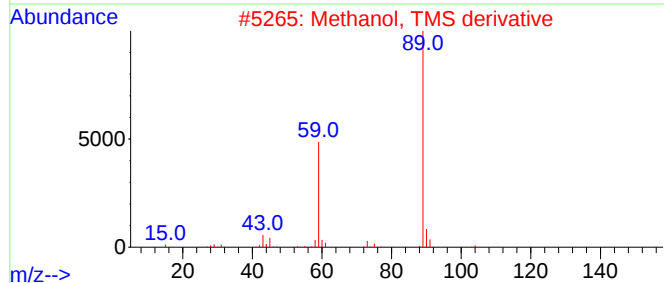
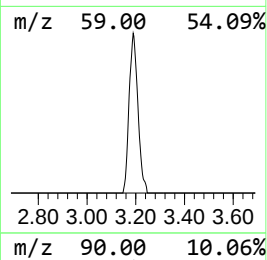
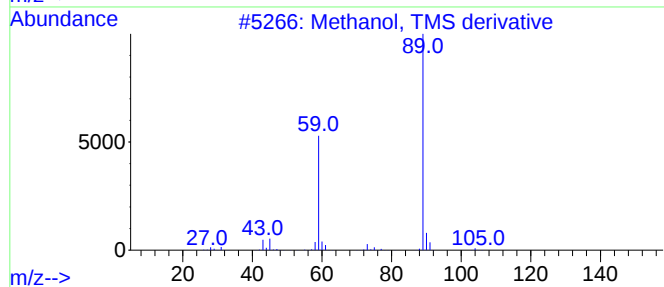
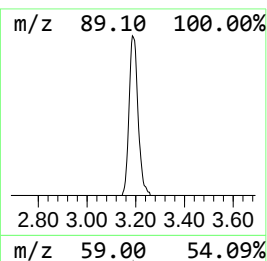
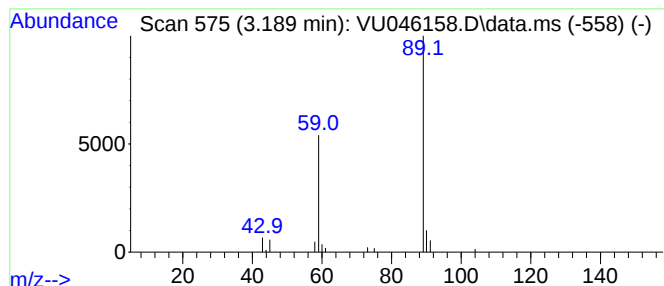
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Methanol, TMS derivative Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.189	2.99 ug/L	32443	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	91
2			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	90
3			Methanol, TBDMS derivative	146	C7H18OSi	1000364-10-7	83
4			Ethyl(dimethyl)methoxysilane	118	C5H14OSi	052686-75-6	74
5			Silane, (2-methoxyethyl)trimethyl-	132	C6H16OSi	018173-63-2	64



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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methanol, TMS d...	3.189	3.0	ug/L	32443	1	6.250	543382	50.0